

Hot Brownian Carriers in the Langevin Picture: Application to a simple model for the Gunn Effect in GaAs.

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We consider a charged Brownian gas under the influence of external, static and uniform electric and magnetic fields, immersed in a uniform bath temperature. We obtain the solution for the associated Langevin equation, and thereafter the evolution of the nonequilibrium temperature towards a nonequilibrium (hot) steady state. We apply our results to a simple yet relevant Brownian model for carrier transport in GaAs. We obtain a negative differential conductivity regime (Gunn effect) and discuss and compare our results with experimental results.

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1: Introduction

The ubiquitous Brownian motion remains an outstanding paradigm in modern physics. Some representative, but by no means an exhaustive list of general references ("founding papers", reviews and applications) are presented in [1-19]. Here we present the Langevin formulation for a Brownian carrier in uniform and static external fields. Some recent work on charged Brownian particles is referenced in [20-47]. In our previous work on this matter, our approach hinged on the resolution of Kramers and/or Smoluchowski equations [24,26,28,45,46,47], and recently we began to tackle Langevin's formulation of this problem [47]. Here we explore the latter, in order to study the relaxation of the Brownian carrier towards a steady state, given electrical and magnetic external static and uniform fields. In section 2 we present the solution of Langevin's equation including the above mentioned fields. In section 3 we present our results for the nonequilibrium temperature relaxation to the "hot" steady state temperature (as modified by the electric and magnetic fields). The computed final "hot" regime temperature is compared to long time existing results ([48] with no magnetic field present) and with our previous results, with the magnetic field contribution, via Kramers and Smoluchowski equations [26,28,45]. In section 4 we present an application, namely a simple yet relevant Brownian model (with no adjustable parameters) for GaAs carrier mobility [49-56]. The multivalley band structure, and the "hot" carrier steady state temperature obtained in the previous section are the essential ingredients for the appearance of a negative differential conductivity regime, in good quantitative agreement with well known experimental results. Furthermore our model incorporates the magnetic field contribution hitherto not considered. Finally, in section 6 we present our concluding remarks and outline further work.

2: Langevin equation for a Brownian charged particle

We briefly present the Langevin formalism for a free charged Brownian particle [10-12,18,19], with mass m , and charge q immersed in an homogeneous thermal reservoir at temperature T_R . It is essentially Newton's equation for the particle with two contributing forces: the

first, a systematic dissipative force Stokes like (linear in the particle's velocity) and the second a rapidly fluctuating random force,

$$m \frac{d\mathbf{v}}{dt} = \mathbf{F}_S + \mathbf{F}^r = -\gamma \mathbf{v} + \mathbf{F}^r(t) \quad \tau = \frac{m}{\gamma} \quad (1)$$

The formal solution is

$$\mathbf{v}(t) = \exp\left(-\frac{t}{\tau}\right) \mathbf{v}^0 + \frac{1}{m} \int_0^t dt_1 \exp\left(-\frac{t_1-t}{\tau}\right) \mathbf{F}^r(t_1) \quad (2)$$

with initial condition $\mathbf{v}^0 = \mathbf{v}(0)$ and τ the collision time. The random force has solely statistical properties: zero average and white noise correlations, given by the averages

$$\langle \mathbf{F}^r(t) \rangle = \mathbf{0} \quad \langle F_i^r(t_1) F_j^r(t_2) \rangle = 2 \frac{m}{\tau} k_B T_R \delta_{ij} \delta(t_1 - t_2) \quad (3)$$

where the correlation strength is such that the asymptotic average kinetic energy satisfies the equipartition theorem, in thermal equilibrium with the thermal reservoir (fluctuation dissipation theorem), and given by

$$\frac{1}{2} m \langle \mathbf{v}^2(t \rightarrow \infty) \rangle = \frac{3}{2} k_B T_R = \frac{1}{2} m V_T^2 \quad (4)$$

Following [28,45,46,47] (and with a slightly different notation) we now consider the Brownian carrier (charged particle) under the influence of homogeneous external, time independent, electric and magnetic fields; the electric contribution is given by $\mathbf{F}_{\text{elec}} = q\mathbf{E}$ and the magnetic contribution (Lorentz's velocity dependent force) $\mathbf{F}_{\text{mag}} = \frac{1}{c} q \mathbf{v} \times \mathbf{B}$. The total external force is given by

$$\mathbf{F}(\mathbf{v}) = \mathbf{F}_{\text{elec}} + \mathbf{F}_{\text{mag}}(\mathbf{v}) = q\mathbf{E} - m\boldsymbol{\omega} \times \mathbf{v} \quad \boldsymbol{\omega} = \frac{q}{mc} \mathbf{B} \quad (5)$$

Let us define a tensorial Stokes force by adding the Lorentz contribution to the usual Stokes force, as

$$\mathbf{F}_{\text{TS}} = -\gamma \mathbf{v} - m\boldsymbol{\omega} \times \mathbf{v} = -m\boldsymbol{\Lambda}^{-1} \mathbf{v} \quad (6)$$

where ω is the usual cyclotron frequency, the magneto mobility tensor is $\mathbf{M} = m^{-1}\mathbf{\Lambda}$ with $\mathbf{\Lambda}$ a tensorial collision time, that can be cast into the form (when operating over an arbitrary vector \mathbf{V})

$$\mathbf{\Lambda}(\tau, \omega)\mathbf{V} = \tau \frac{\mathbf{V} + \tau \mathbf{V} \times \omega + \tau^2 \omega (\omega \cdot \mathbf{V})}{1 + \tau^2 \omega^2} \quad (7)$$

In particular notice the familiar form for the case $\mathbf{B} = B\hat{z}$

$$\mathbf{\Lambda}(\tau, \omega) = \frac{\tau}{1 + \tau^2 \omega^2} \begin{pmatrix} 1 & \tau\omega & 0 \\ -\tau\omega & 1 & 0 \\ 0 & 0 & 1 + \tau^2 \omega^2 \end{pmatrix} \quad (8)$$

By defining such a tensorial Stokes force, Langevin's equation now reads

$$m \frac{d\mathbf{v}}{dt} = -m\mathbf{\Lambda}^{-1}\mathbf{v} + q\mathbf{E} + \mathbf{F}^r(t) \quad (9)$$

with formal solution [57-60]

$$\mathbf{v}(t) = \exp(-\mathbf{\Lambda}^{-1}t) \mathbf{v}^0 + \mathbf{\Lambda} (1 - \exp(-\mathbf{\Lambda}^{-1}t)) \frac{q\mathbf{E}}{m} + \frac{1}{m} \int_0^t dt_1 \exp(\mathbf{\Lambda}^{-1}(t_1 - t)) \mathbf{F}^r(t_1) \quad (10)$$

Using Cayley-Hamilton theorem, and Putzer [59] and Apostol [60] results, after a lengthily but straight forward calculation we obtain

$$\exp(\mathbf{\Lambda}^{-1}t) = a_0(t) + a_1(t)\mathbf{\Lambda}^{-1} + a_2(t)\mathbf{\Lambda}^{-2} \quad (11)$$

$$= \exp\left(\frac{t}{\tau}\right) \left(1 + \frac{1}{\omega^2}(\mathbf{\Lambda}^{-1} - \tau^{-1})^2(1 - \cos \omega t) + \frac{1}{\omega}(\mathbf{\Lambda}^{-1} - \tau^{-1}) \sin \omega t\right) \quad (12)$$

3: Evolution of the Effective (nonequilibrium) temperature towards a hot steady state.

Let us define the nonequilibrium effective temperature $T_{\text{ef}}(t)$ as

$$\frac{3}{2}k_B T_{\text{ef}}(t) = \frac{1}{2}m \langle \mathbf{v}^2(t) \rangle \quad (13)$$

and consider "thermal like" initial velocity conditions, *i.e.* configurational averages $\langle \rangle_c$ over initial velocities are given by Maxwell like distributions

$$\langle \mathbf{v}^0 \rangle_c = \mathbf{0} \quad \frac{1}{2}m \langle v_i^0 v_j^0 \rangle_c = \frac{1}{2}k_B T_0 \delta_{ij} \quad (14)$$

where $T_0 < T_R$ ($T_0 > T_R$) defines cold (hot) initial distributions. Furthermore we define dimensionless electric and magnetic fields \mathbf{e} and \mathbf{b} as

$$\mathbf{e}^2 = \frac{\tau^2 q^2 \mathbf{E}^2}{3mk_B T_R} = \left(\frac{\mathbf{V}_E}{V_T} \right)^2 \quad \mathbf{V}_E = \frac{q\tau \mathbf{E}}{m} \quad (15)$$

$$\mathbf{b} = \tau \boldsymbol{\omega} \quad \mathbf{eb} = eb \cos \theta \quad \omega = |\boldsymbol{\omega}| \quad (16)$$

and θ the angle between fields. Furthermore we introduce a dimensionless time in collision time units and denoted hereafter as $t = t/\tau$. Finally, by considering equation (3), some trivial integration and basic vector and matrix algebra, the expression for the effective temperature is given by

$$T_{\text{ef}}(t) = T_0 \exp(-2t) + T_R (1 - \exp(-2t)) + T_R \mathbf{e}^2 \left(\frac{1 + b^2 \cos^2 \theta}{1 + b^2} + \Gamma_1(t) + \Gamma_2(t) \right) \quad (17)$$

with

$$\Gamma_1(t) = \frac{2 \exp(-t)}{1 + b^2} \left(\left(\cos bt + \frac{2b}{1 + b^2} \sin bt \right) \sin^2 \theta + \cos^2 \theta \right) \quad (18)$$

$$\Gamma_2(t) = \exp(-2t) \left(1 + b^2 \cos^2 \theta + \frac{4b}{(1 + b^2)^2} \cos bt \sin bt \sin^2 \theta + \cos^2 \theta \right) \quad (19)$$

The Brownian carrier gas evolves towards a stationary state with a nonequilibrium temperature greater than the reservoir temperature, thereby the name hot carrier.

$$\Theta = \frac{T_{\text{ef}}(t \rightarrow \infty)}{T_R} = 1 + \left(\frac{1 + b^2 \cos^2 \theta}{1 + b^2} \right) \mathbf{e}^2 \quad (20)$$

This result includes the magnetic field effect. In the Kramers Smoluchowski scheme [26,28,45] we derived the expression

$$\Theta_K = \frac{T_{\text{ef}}^{\text{Kramers}}(t \rightarrow \infty)}{T_R} = 1 - \frac{1}{t} + \left(\frac{1 + b^2 \cos^2 \theta}{1 + b^2} \right) \left(\mathbf{e} - \tau V_T \frac{\nabla n(\mathbf{x})}{n(\mathbf{x})} \right)^2 \quad (21)$$

where a long tail ($1/t$ non exponential tail, see also [25]) and the spatial inhomogeneity of the carrier's distribution corrects the electric field contribution. Both the long tail and the density diffusive effect smears out at longer times rendering both expressions equivalent. We believe equations (20) and (21) represent novel results at least in the Brownian context, as far as the magnetic field contribution is concerned. Shockley obtained an expression for the hot carrier temperature [48-50] for null magnetic field and in agreement with our result in equation (20) for $b = 0$. The absence of the electric field renders the equilibrium (reservoir) temperature, regardless of the magnetic field value. For non zero electric field values, the magnetic field modulates the hot carrier's temperature with maximum value for parallel fields (independent of the magnetic field value) and minimum value for perpendicular fields.

Figures 1 to 5 we plot the effective temperature evolution, with unit time given by the collision time constant τ . Solid lines represent the zero magnetic field and dashed lines the magnetic and angle value on display in each figure. The reservoir temperature is fixed at 400⁰K and two values are chosen for T_0 namely 200⁰K (cold) and 600⁰K (hot) initial velocity distributions. The cold (hot) cases are the lower (upper) curves starting at $t = 0$. We observe that after a few collision time units the carrier's temperature reaches the stationary value that decreases as the magnetic field deviates from the parallel configuration, similarly for the non parallel case as the magnetic field increases. The transient effects are damped oscillations, a larger effect for intermediate magnetic field values. The dimensionless field

values where chosen from typical material parameters for GaAs (see next section), rendering:
 $e = 1$ corresponds to 1000 volts/cm and $b = 1$ corresponds to one Tesla.

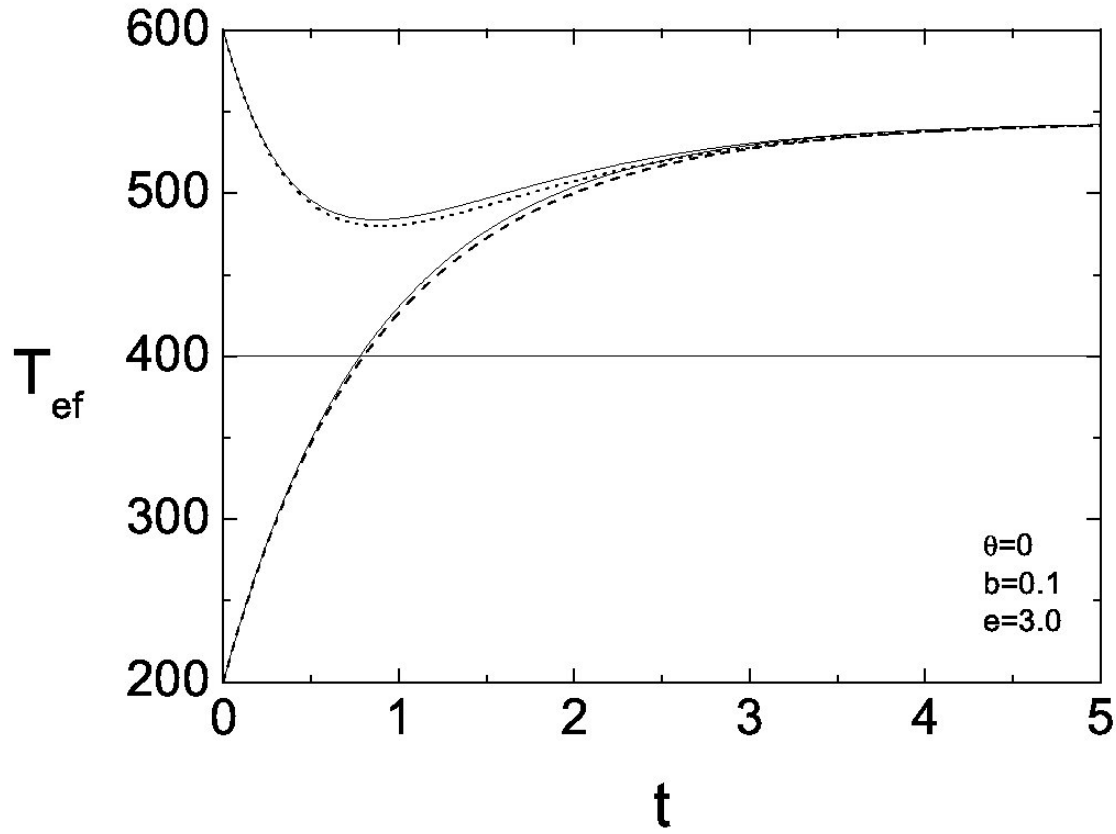


Figure 1: *Effective temperature versus time, electric field $e = 3.0$. Solid lines represent the zero magnetic field case $b = 0$, dashed lines the case $b = 0.1$, $\theta = 0$. Hot initial condition given by $T_{ef}(0) = 600^0K$ and cold initial condition by $T_{ef}(0) = 200^0K$. See main text for time and field units.*

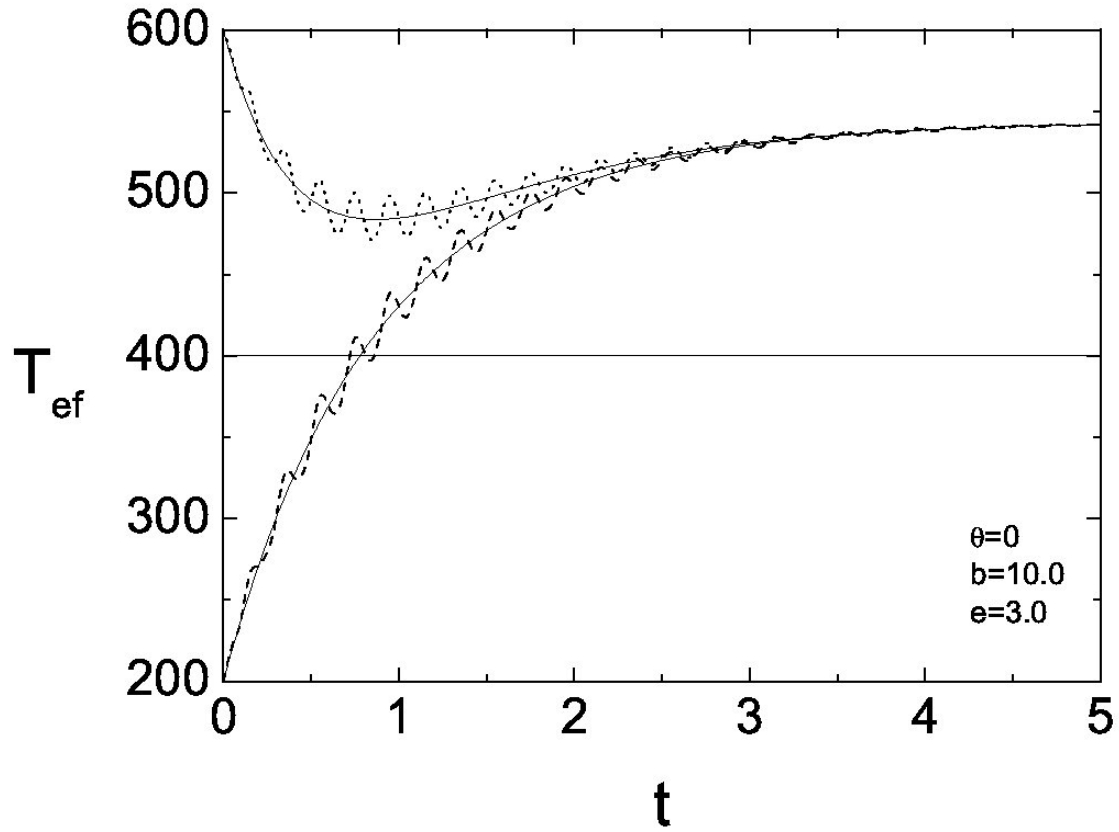


Figure 2: *Effective temperature versus time, electric field $e = 3.0$. Solid lines represent the zero magnetic field case $b = 0$, dashed lines the case $b = 10.0$, $\theta = 0$. Hot initial condition given by $T_{ef}(0) = 600^0K$ and cold initial condition by $T_{ef}(0) = 200^0K$. See main text for time and field units.*

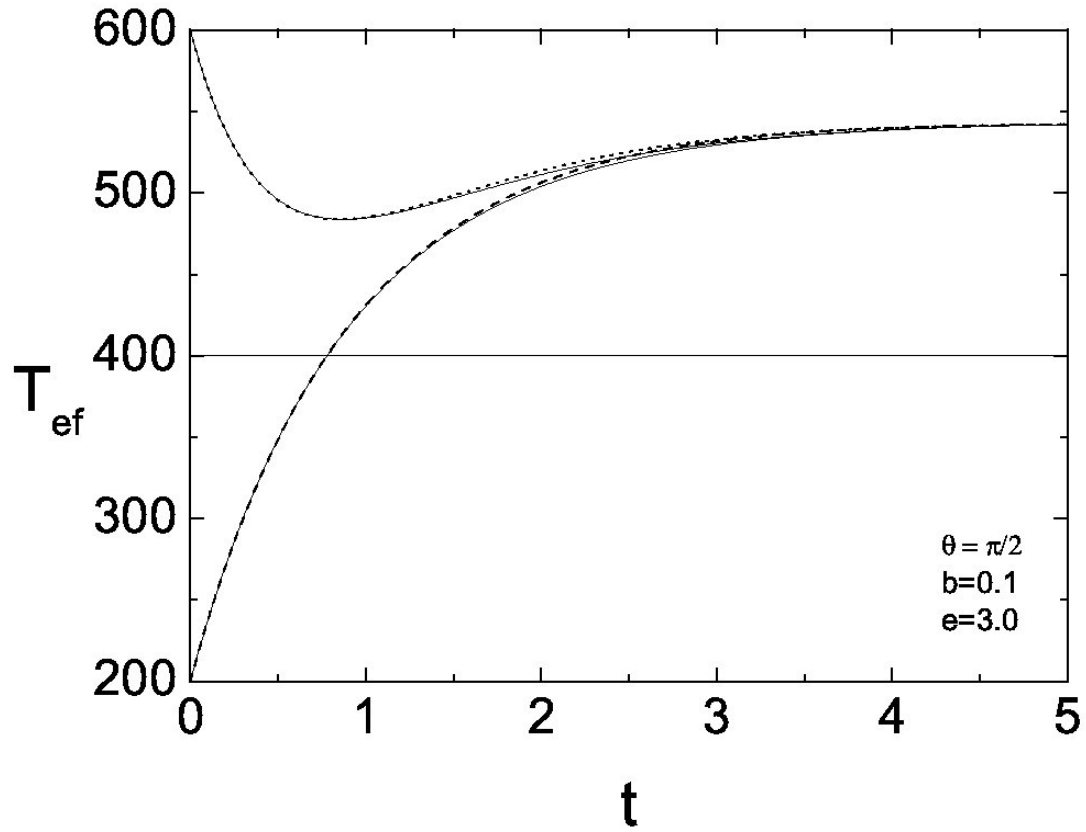


Figure 3: *Effective temperature versus time, electric field $e = 3.0$. Solid lines represent the zero magnetic field case $b = 0$, dashed lines the case $b = 0.1$, $\theta = \pi/2$. Hot initial condition given by $T_{ef}(0) = 600^0K$ and cold initial condition by $T_{ef}(0) = 200^0K$. See main text for time and field units.*

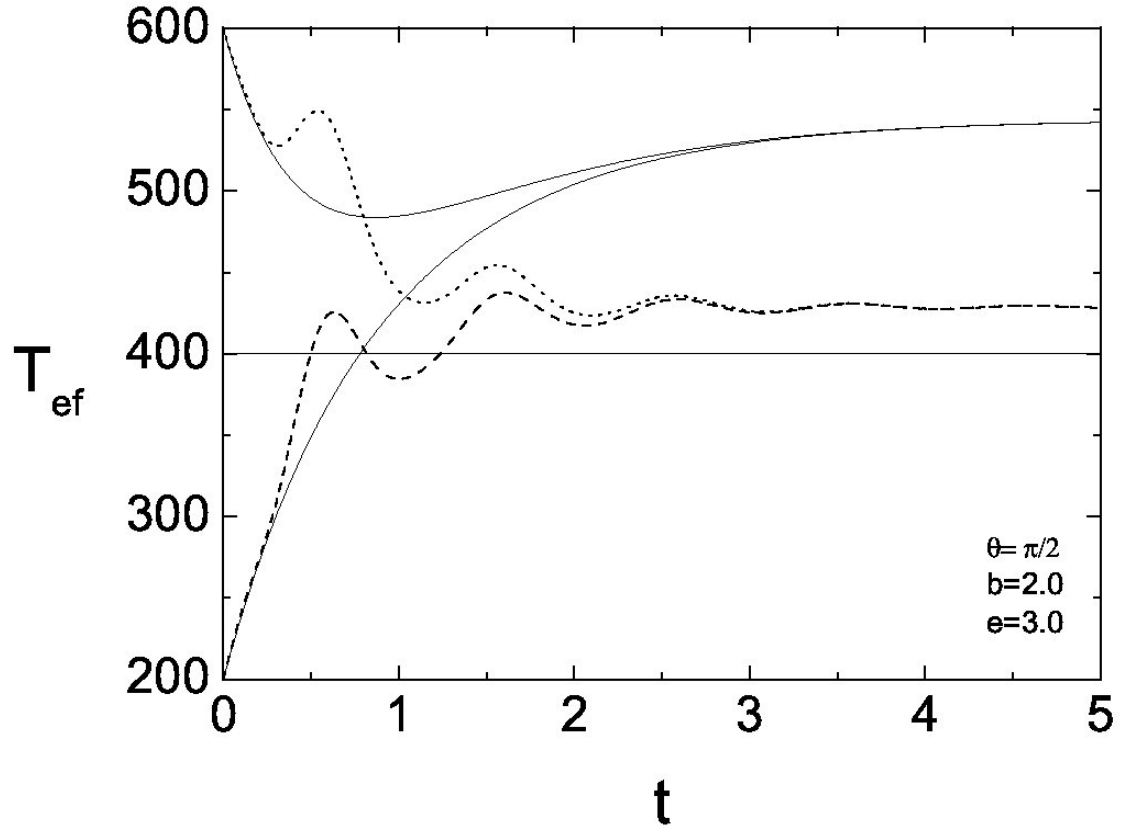


Figure 4: *Effective temperature versus time, electric field $e = 3.0$. Solid lines represent the zero magnetic field case $b = 0$, dashed lines the case $b = 2.0$, $\theta = \pi/2$. Hot initial condition given by $T_{ef}(0) = 600^0K$ and cold initial condition by $T_{ef}(0) = 200^0K$. See main text for time and field units.*

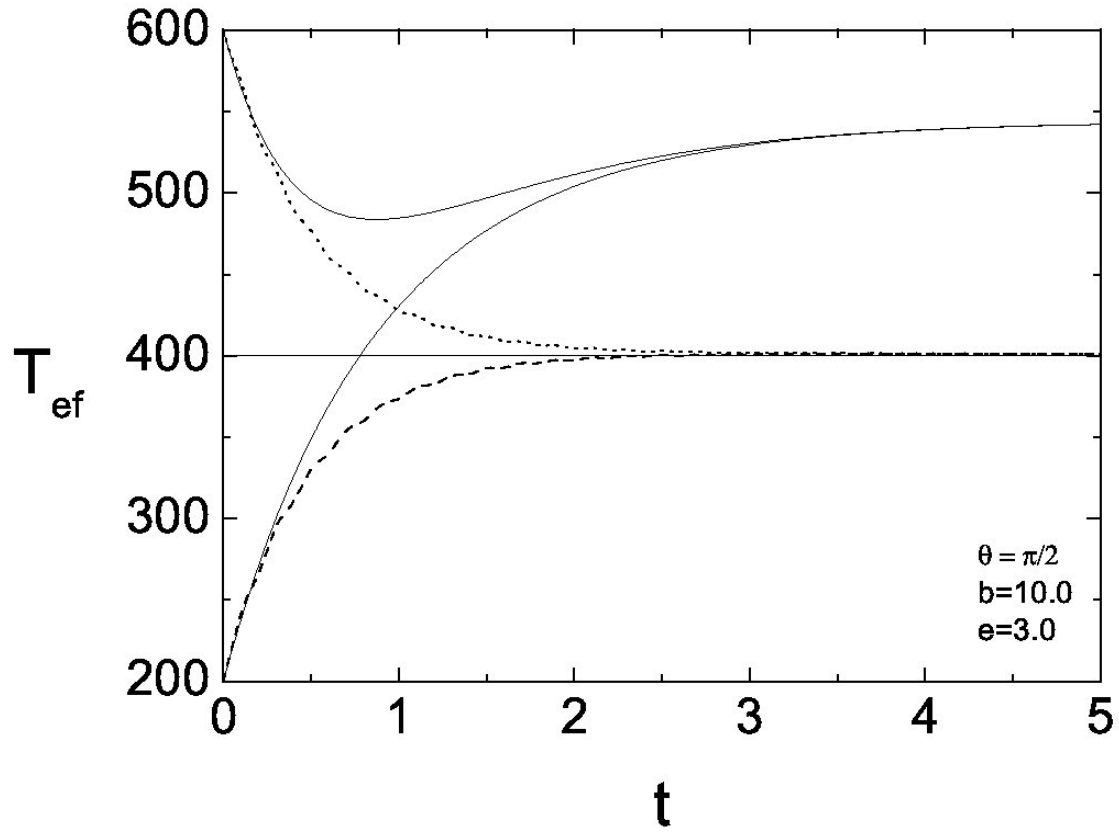


Figure 5: *Effective temperature versus time, electric field $e = 3.0$. Solid lines represent the zero magnetic field case $b = 0$, dashed lines the case $b = 10.0$, $\theta = \pi/2$. Hot initial condition given by $T_{ef}(0) = 600^0K$ and cold initial condition by $T_{ef}(0) = 200^0K$. See main text for time and field units.*

4: Simple Brownian carrier model for GaAs. Negative differential conductivity.

Gallium arsenide (GaAs) is a compound of the elements Gallium and Arsenic. It is a III/V semiconductor, and is used in the manufacture of devices such as microwave frequency integrated circuits, monolithic microwave integrated circuits, infrared light-emitting diodes, laser diodes, solar cells and optical windows. The band structure consists of a multivalley landscape. Based on data from references [49-56] we model the electron mobility μ (proportional to the drift velocity V_D), combining the high mobility Γ valley with low mobility L valley (six satellite valleys per Γ type valley). The carrier mobility is obtained via standard canonical average restricted to these two type of valleys,

$$\mu = \frac{\mu_\Gamma P_\Gamma + \mu_L P_L}{P_\Gamma + P_L} \quad (22)$$

with the usual expressions as given in the literature [49-56]

$$\mu_\alpha = \mu_0 \sqrt{\frac{1}{m_\alpha T}} \quad P_\alpha \sim g_\alpha m_\alpha^{3/2} \exp\left(-\frac{E_\alpha}{k_B T}\right) \quad \alpha = \Gamma, L \quad (23)$$

where μ_0 is proportional to a typical mean velocity equation (10) and with relevant typical parameters given by: $g_L = 6g_\Gamma$, $m_L \simeq 10m_\Gamma$ and $\Delta = E_L - E_\Gamma \simeq 0.3\text{eV}$. At room temperature 300^0K we have $\Delta/k_B T_R \simeq 12$. The drift velocity (mobility times electric field) is computed in the electric field direction as (in arbitrary units).

$$V_D = \frac{\mu}{\mu_0} \frac{\mathbf{v}(t \rightarrow \infty) \cdot \mathbf{E}}{|\mathbf{E}|} \quad (24)$$

With typical values for GaAs we compute the last equation using equations (10) and (22) yielding the material parameter free equations

$$V_D = \frac{1}{\sqrt{\Theta}} \left(\frac{1 + 60 \exp(-12\Theta^{-1})}{1 + 130 \exp(-12\Theta^{-1})} \right) \Omega |\mathbf{e}| \quad (25)$$

$$\Omega = \frac{1 + \mathbf{b}^2 \cos^2 \theta}{1 + \mathbf{b}^2} \quad (26)$$

$$\Theta = 1 + 0.04\Omega \mathbf{e}^2 \quad (27)$$

notice that for zero gap we obtain a typical Caughey Thomas [56] expression for the mobility.

$$V_D^{\Delta=0} = \frac{0.47\Omega}{\sqrt{1 + 0.04\Omega\epsilon^2}} |\mathbf{e}| \quad (28)$$

Caughey Thomas mobility modeling is a non linear phenomenological fitting procedure. Our general result is linear in the electric field (in the linear regime, the current is a transport coefficient times the field), incorporates the magnetic field, and the nonlinear electric field dependence is due to the non equilibrium temperature intrinsic field dependence. As mentioned in the previous section, the dimensionless field values were chosen from typical material parameters for GaAs, rendering: $e = 1 \rightarrow E = 1000$ volts/cm and $b = 1 \rightarrow B = 1$ Tesla.

In Figures 6 to 9 we plot the drift velocity in arbitrary units versus electric field. The solid upper line is the zero magnetic field case and the lower solid lines is the corresponding Caughey Thomas case ($\Delta = 0$). The dashed lines correspond to the angle and magnetic field values on display in each figure, the dashed lines maximum decreases as the magnetic field value increases. For all cases presented we find a region of negative differential conductivity (Gunn effect)

$$\frac{dV_D(e)}{de} < 0$$

for electric field larger than the critical value $e_c \sim 4000$ Volts/cm, $\left(\frac{dV_D(e_c)}{de_c} = 0\right)$ as it is well known for this compound [49,50,52-54]. From Figures 6-9 and considering equations (25-27), as the magnetic field value is increased we notice that $e_c(b)$ increases and $V_D(e_c(b))$ decreases while the effective temperature $\Theta(e_c(b), b, \theta)$ decreases. This pattern becomes more pronounced as we move from parallel fields towards perpendicular fields. The available experimental data for a related compound [55], where the negative differential conductivity region was probed with a magnetic field, seems to corroborate our findings, in a very qualitative fashion. In the higher electric field regions, say $e \gtrsim 10$ where our results deviates from the experimental data, the effective temperature Θ is very large, quite probably other scattering mechanisms should be incorporated, rendering a more involved temperature dependence for the mobility (see equation (23)), and more than one collision time constant

should be considered. We include very large magnetic field values solely to probe the pattern described above.

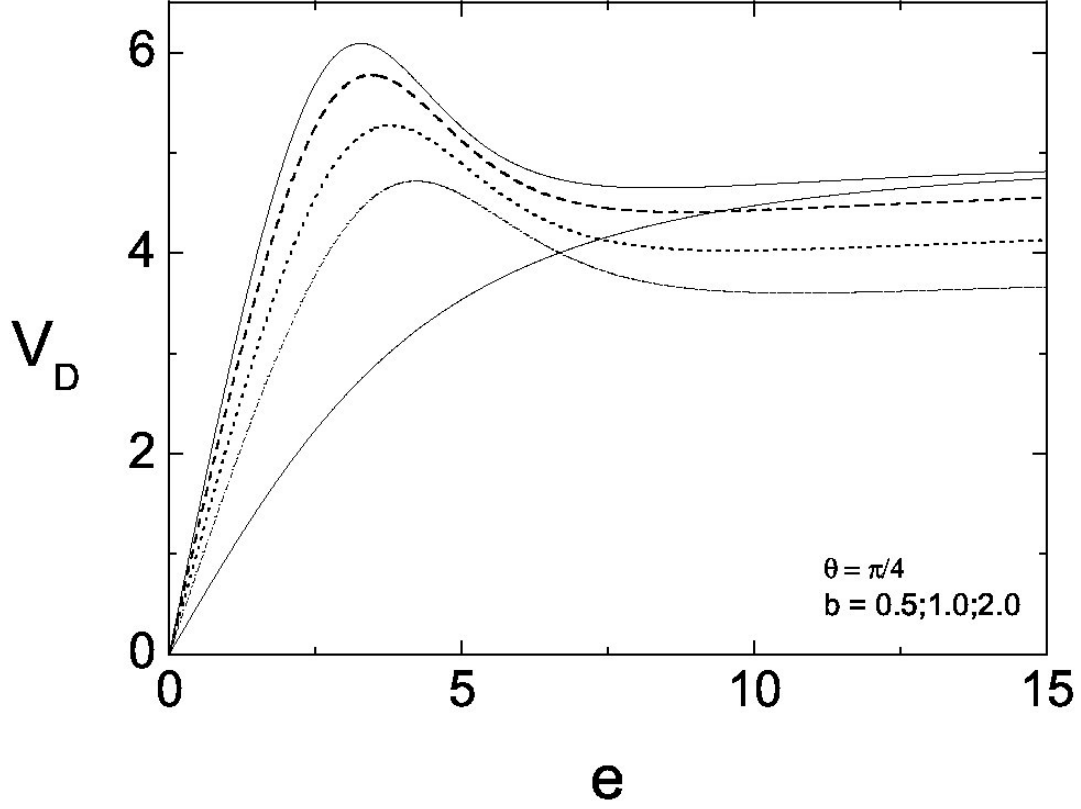


Figure 6: *Drift velocity versus electric field. Upper solid line for zero magnetic field (or arbitrary magnetic field with $\theta = 0$). Dashed lines in decreasing order for $b = 0.5, 1.0$ and 2.0 , with $\theta = \pi/4$. Lower solid line case of null gap and zero magnetic field. See main text for velocity and field units.*

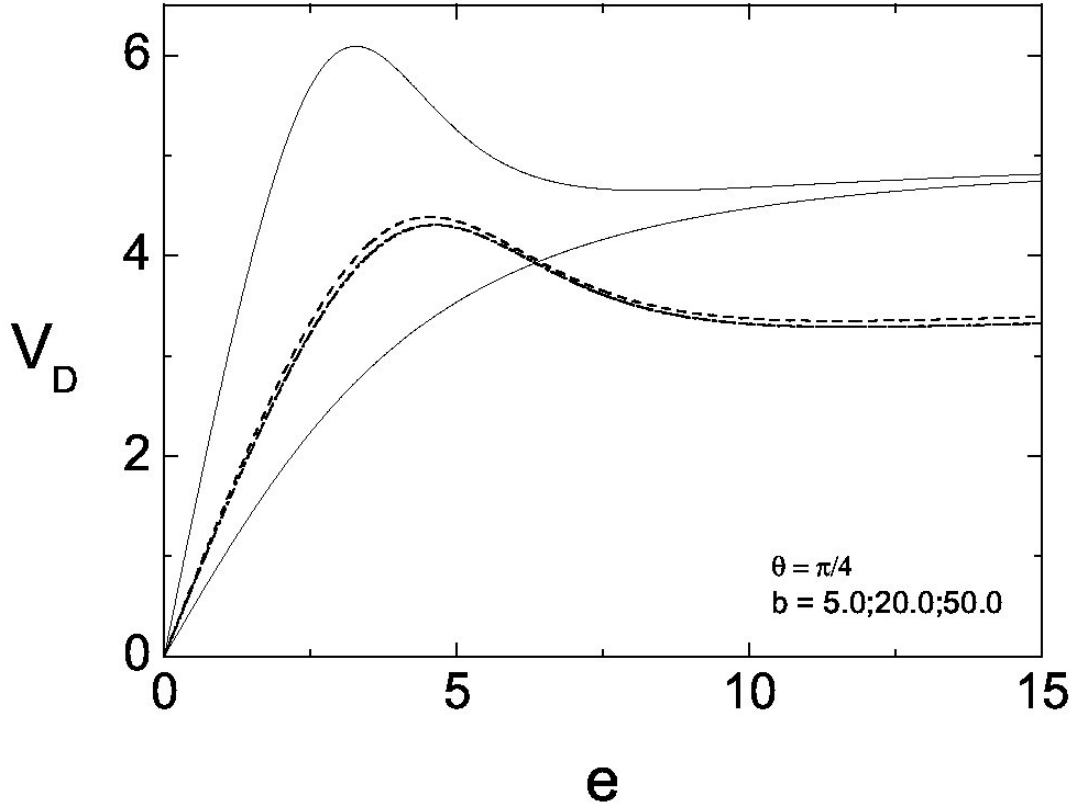


Figure 7: *Drift velocity versus electric field. Upper solid line for zero magnetic field (or arbitrary magnetic field with $\theta = 0$). Dashed lines in decreasing order for $b = 5.0, 20.0$ and 50.0 (the last two cases overlap on the scale used), with $\theta = \pi/4$. Lower solid line case of null gap and zero magnetic field. See main text for velocity and field units.*

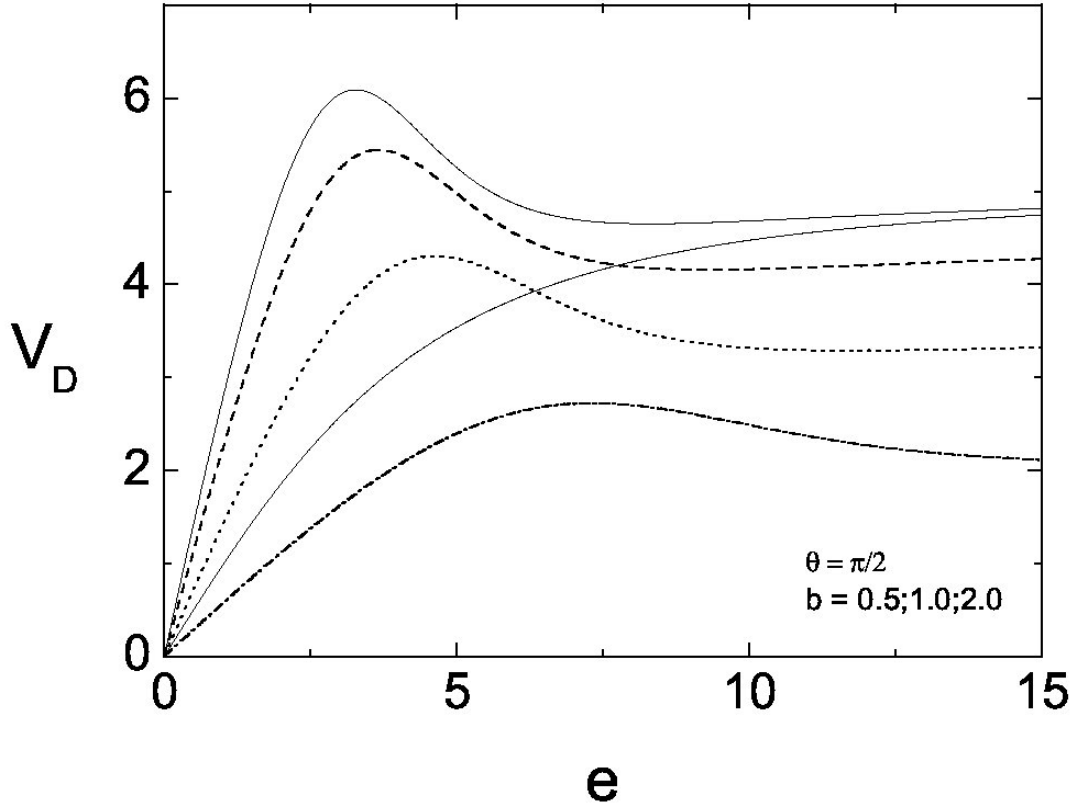


Figure 8: *Upper solid line for zero magnetic field (or arbitrary magnetic field with $\theta = 0$). Dashed lines in decreasing order for $b = 0.5, 1.0$ and 2.0 , with $\theta = \pi/2$. Lower solid line case of null gap and zero magnetic field. See main text for velocity and field units.*

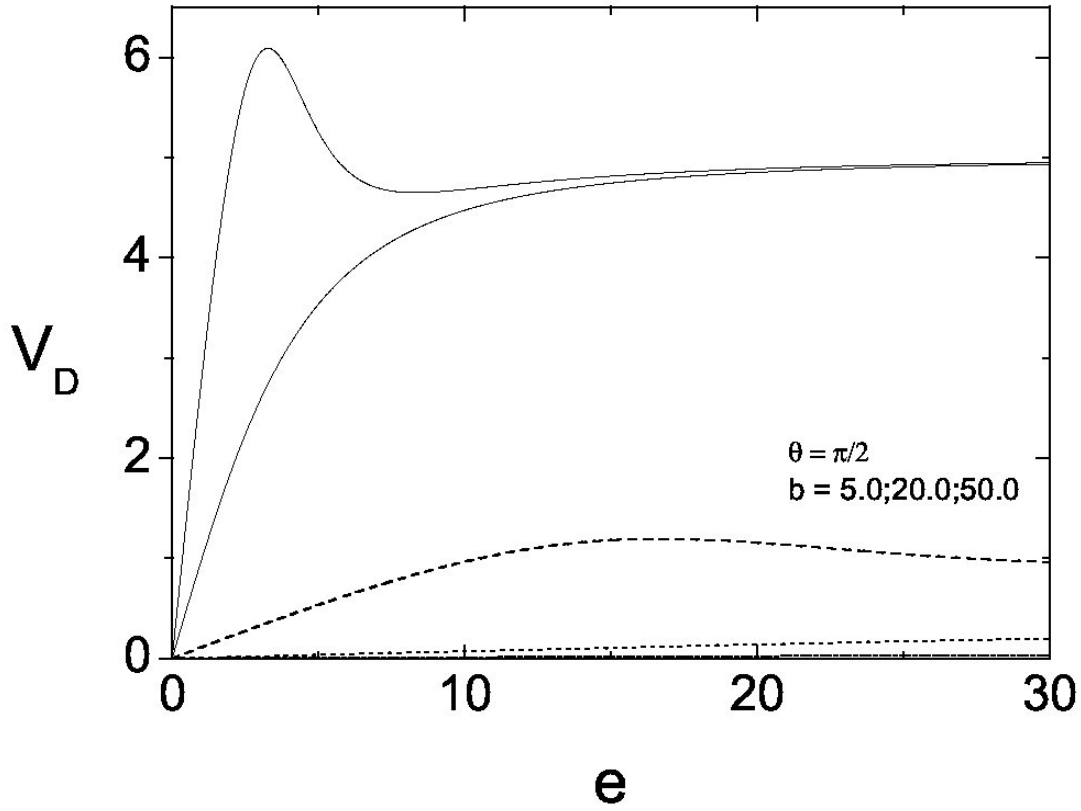


Figure 9: *Drift velocity versus electric field. Upper solid line for zero magnetic field (or arbitrary magnetic field with $\theta = 0$). Dashed lines in decreasing order for $b = 5.0, 20.0$ and 50.0 (the last case almost indistinguishable from the e axis, on the scale used), with $\theta = \pi/2$. Lower solid line case of null gap and zero magnetic field. See main text for velocity and field units.*

5: Concluding remarks

We presented the Langevin formulation for a Brownian carrier under uniform and static external electric and magnetic fields. From the solution to the associated Langevin equation, we computed the relaxation of the carrier's effective (nonequilibrium) temperature towards a (hot) steady state regime with a nonequilibrium field dependent temperature. The latter was compared with well known existing results. We believe our present result in the Langevin as well as our previous results in the Kramers Smoluchowski scheme, incorporate the effect of the magnetic field hitherto not considered. Then we presented a simple yet relevant Brownian model to account for the negative differential conductivity behavior on the GaAs compound, again incorporating the magnetic field effects hitherto not considered. Discussions of results and Figures are presented at the end of sections 3 and 4.

Our future work includes the incorporation of diffusive effects on the effective temperature, as discussed in section 3, the inclusion of other scattering mechanisms into the mobility as discussed in section 4, and incorporate within the Langevin Formalism chemical reactions [61-62] and photovoltaic effects [63] as discussed for example in [45] within the Kramers Smoluchowski context.

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